CHARACTERIZING MOLECULAR STRUCTURE BY COMBINING EXPERIMENTAL MEASUREMENTS WITH DENSITY FUNCTIONAL THEORY COMPUTATIONS

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In this talk, the power and synergy of combining experimental measurements with density functional theory computations as a single tool to unambiguously characterize the molecular structure of complex atomic systems is shown. Here, we bring three beautiful cases where the interaction between the experiment and theory is in very good agreement for both finite and extended systems: 1) Characterizing Metal Coordination Environments in Porous Organic Polymers: A Joint Density Functional Theory and Experimental Infrared Spectroscopy Study[b]; 2) Characterization of Rhenium Compounds Obtained by Electrochemical Synthesis After Aging Process[c]; and 3) Infrared Study of $H(D)_2$ + $Co_4{}^+$ Chemical Reaction: Characterizing Molecular Structures.

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